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ABSTRACT

Diffusion coefficients are computed for a typical ZPPR lattice cell using the methods of Benoist and Bonalumi. It is noted that the diffusion coefficients, D_x, for leakage normal to the plates, as defined by Benoist and by Bonalumi, are both double-valued. The spread between Benoist's x-diffusion coefficients is, in the ZPPR cell, half as large as the difference between D_x and D_y. Bonalumi's x-diffusion coefficients are much farther apart, the interval between them being considerably larger than the difference between D_x and D_y. Neither the Benoist nor the Bonalumi method yields homogenized diffusion coefficients which preserve fluxes, reaction rates, or eigenvalues. A modified definition of homogenized diffusion coefficients is proposed for one-group problems. The modified parameters are defined so as to guarantee that eigenvalues are preserved in the homogenization process. It is felt that generalization to the multigroup case will not be difficult. The relation between the new diffusion coefficients and the Benoist coefficients is discussed.

I.   INTRODUCTION

In published work on the analysis of ZPPR critical experiments[1] anisotropic diffusion has, so far, been neglected. Such an approach seems reasonable in a first approximation since, at the high energies where most leakage occurs, the ZPPR fuel plates are optically thin. Recent Argonne calculations indicate, however, that in the range from 1-10 MeV, the diffusion coefficients parallel to and perpendicular to the plate surfaces may differ by as much as 4%, and that in some ZPPR assemblies this difference will induce an 0.8% change in k_{eff}.[2] Thus, while anisotropic diffusion effects in ZPPR criticals are normally not very large, neither are they negligible.

A great many methods are available for the treatment of anisotropic diffusion in heterogeneous assemblies. It is not our intention here, however, to survey all these methods or to elaborate the intricate relations between them. Instead we focus our attention on only two, namely, Benoist's method[3] and the more recently developed method of Bonalumi.[4]

Benoist's method is well-known and has been widely used, apparently with great success. Nevertheless important questions about the accuracy and range of validity of this method remain, and seem to require further attention. One finds, for example, that there is in the literature no detailed analysis of the accuracy of the Benoist method in slab cells like those of the ZPPR lattice. It may be argued that, if Benoist's method is adequate for the treatment of thermal reactor lattices, it must surely be adequate in ZPPR lattices where the fuel is relatively thin and heterogeneity effects are relatively small. But, precisely because the fuel plates are thin, the flux in and near the plates is highly anisotropic[5]

whereas Benoist's method is based on the approximation that it is *iso-tropic*. It seems proper, then, to question the validity of this as well as other Benoist approximations before relying on the Benoist method for the analysis of ZPPR critical assemblies.

A more fundamental question is raised by Bonalumi,[4] who objects to Benoist's definition of effective diffusion coefficients, and proposes another. Benoist's and Bonalumi's methods do not differ *radically* from each other, and they share with other methods some seemingly universal features. Apparently all methods discussed in the literature on aniso-tropic diffusion assume, first, that in the lattice an overall buckling, $\underline{B}$, is superimposed on a periodic flux; secondly, that the leakage asso-ciated with this buckling can be expanded in a Taylor series in the com-ponents of $\underline{B}$; and, finally, that the buckling is small enough so that only leading terms in such a series need be retained. But the methods of Benoist and Bonalumi, despite these similarities, yield diffusion coefficients which, in a typical ZPPR lattice, are substantially dif-ferent from each other. Clearly, then, one is called upon to establish a rationale for choosing between these methods before either is used for the analysis of ZPPR critical assemblies.

It should be noted that *both* the Benoist and Bonalumi definitions give us double-valued diffusion coefficients, though this point seems to have been overlooked in the literature. We shall see that the spread between the permissable values of D normal to the plates is rather large if we accept Bonalumi's definition. If instead, we accept Benoist's definition, this spread becomes considerably smaller.

Both the Bonalumi and Benoist definitions of D seem somewhat arbi-trary. We shall show that, in a nonmultiplying medium, neither yields

fluxes and absorption rates which match those in the original hetero-geneous lattice, and neither gives the right eigenvalue when fission is present. Thus, there seems to be room for still another definition and, in closing, we propose a definition which, in one energy group, *does* give the right eigenvalue. It seems likely that this definition can be reformu-lated easily for multi-energy problems, though this has not yet been done.

II. THE METHODS OF BENOIST AND BONALUMI IN SLAB LATTICES

We begin by deriving Benoist's and Bonalumi's equations specialized to slab lattices. Of course, derivations for general geometries already exist in the literature. It is our purpose, in rederiving these equa-tions, to develop our notation and to exhibit all implied approximations as clearly as possible.

In one energy, with isotropic scattering, the transport equation takes the form

$$\hat{\Omega} \cdot \nabla F(\underline{r},\hat{\Omega}) + \Sigma_t F(\underline{r},\hat{\Omega}) = (1/4\pi)\Sigma_s(\underline{r})\Phi(\underline{r}) + (1/4\pi)S(\underline{r}) \ . \tag{1}$$

We assume that, in the slab lattice,[6]

$$S(\underline{r}) = q(x) \cos (\underline{B} \cdot \underline{r}) = R\{q(x) e^{i\underline{B}\cdot\underline{r}}\} \ , \tag{2}$$

where $q(x)$ has the periodicity of the lattice. Correspondingly,

$$F(\underline{r},\hat{\Omega}) = R\{f(x,\hat{\Omega}) e^{i\underline{B}\cdot\underline{r}}\} \ , \tag{3}$$

and

$$\Phi(\underline{r}) = R\{\chi(x) e^{i\underline{B}\cdot\underline{r}}\} \ , \tag{4}$$

where, again, f and χ have the periodicity of the lattice. Note that f and χ are generally complex. Inserting Eqs. (2), (3), and (4) into Eq. (1), we find that

$$\hat{\Omega} \cdot \nabla f(x,\hat{\Omega}) + \left[\Sigma_t(x) + i(\hat{\Omega} \cdot \underline{B})\right] f(x,\hat{\Omega}) = (1/4\pi)\Sigma_s \chi(x) + (1/4\pi)q(x) \ . \quad (5)$$

Let

$$R(x,\hat{\Omega}) = R\{f(x,\hat{\Omega})\}, \quad I(x,\hat{\Omega}) = I\{f(x,\hat{\Omega})\} \ , \quad (6)$$

$$\rho(x) = R\{\chi(x)\}, \quad \psi(x) = I\{\chi(x)\} \ . \quad (7)$$

Then, from Eqs. (5) and (6),

$$\hat{\Omega} \cdot \nabla R(x,\hat{\Omega}) + \Sigma_t R(x,\hat{\Omega}) = (1/4\pi)\Sigma_s(x)\rho(x) + (1/4\pi)q(x)$$

$$+ (\hat{\Omega} \cdot \underline{B})I(x,\hat{\Omega}) \ , \quad (8)$$

$$\hat{\Omega} \cdot \nabla I(x,\hat{\Omega}) + \Sigma_t I(x,\hat{\Omega}) = (1/4\pi)\Sigma_s(x)\psi(x) - (\hat{\Omega} \cdot \underline{B})R(x,\hat{\Omega}) \ . \quad (9)$$

Now we expand R and I in Taylor series in the two variables B_x and B_y:

$$R(x,\hat{\Omega}) = \sum_{n,m=0}^{\infty} B_x^n B_y^m R^{(n,m)}(x,\hat{\Omega}) \ , \quad (10)$$

$$I(x,\hat{\Omega}) = \sum_{n,m=0}^{\infty} B_x^n B_y^m I^{(n,m)}(x,\hat{\Omega}) \ . \quad (11)$$

It can easily be shown that $I^{(0,0)} = 0$, and that the leading terms in Eqs. (10) and (11) satisfy the equations:

$$\mu \frac{\partial R^{(0,0)}}{\partial x} + \Sigma_t R^{(0,0)} = \frac{\Sigma_s}{4\pi} \int d\hat{\Omega} \ R^{(0,0)} + \frac{1}{4\pi} q(x) \ , \quad (12)$$

$$\mu \frac{\partial I^{(0,1)}}{\partial x} + \Sigma_t I^{(0,1)} = \frac{\Sigma_s}{4\pi} \int d\hat{\Omega}\ I^{(0,1)} - \Omega_y R^{(0,0)} \ , \ \text{(see Ref. 7)} \quad (13)$$

$$\mu \frac{\partial I^{(1,0)}}{\partial x} + \Sigma_t I^{(1,0)} = \frac{\Sigma_s}{4\pi} \int d\hat{\Omega}\ I^{(1,0)} - \mu R^{(0,0)} \ , \quad (14)$$

where

$$\mu \equiv \Omega_x \ .$$

From Eqs. (3), (6), and (7) we see that, to first order in B,

$$F(\underline{r},\hat{\Omega}) = R^{(0,0)} \cos (\underline{B} \cdot \underline{r}) - I_1 \sin (\underline{B} \cdot \underline{r}) \ , \quad (15)$$

$$I_1 \equiv B_x I^{(1,0)} + B_y I^{(0,1)} \ . \quad (16)$$

The current, $\underline{J}$, is, by definition, given by the expression

$$\underline{J} = \int \hat{\Omega}\ d\hat{\Omega} \left[R^{(0,0)} \cos (\underline{B} \cdot \underline{r}) - I_1 \sin (\underline{B} \cdot \underline{r}) \right]$$

$$= \underline{J}_0 \cos (\underline{B} \cdot \underline{r}) + \underline{J}_1 \sin (\underline{B} \cdot \underline{r}) \ , \quad (17)$$

where

$$\underline{J}_0 \equiv \int \hat{\Omega}\ d\hat{\Omega}\ R^{(0,0)} \ , \qquad \underline{J}_1 \equiv -\int \hat{\Omega}\ d\hat{\Omega}\ I_1 \ .$$

Let x_L and x_R be, respectively, the left- and right-hand cell boundaries.[8] Since we are dealing with a lattice consisting of infinite slabs, we may define the upper and lower horizontal boundaries arbitrarily. In any case the net leakage, L, out of the cell is given by the expression

$$L = \int_{cell} \nabla \cdot \underline{J}\ dv \ . \quad (18)$$

Now we note, first, that $R^{(0,0)}$ satisfies reflecting boundary conditions at x_L and x_R. Secondly (since $R^{(0,0)}$ is the flux in the cell when $\underline{B} = 0$), it is clear that $\underline{J}_0$ lies in the x direction, i.e., $\underline{J}_0 = \underline{J}_{0x}$. Therefore,

$$\int_{cell} \nabla \cdot \left[\underline{J}_0 \cos (\underline{B} \cdot \underline{r}) \right] dv = \int_{cell} (\partial/\partial x) \left[\underline{J}_0 \cos (\underline{B} \cdot \underline{r}) \right] = 0 . \quad (19)$$

Thus,

$$L = \int_{cell} \nabla \cdot \left[\underline{J}_1 \sin (\underline{B} \cdot \underline{r}) \right] dV . \quad (20)$$

Carrying out the differentiation indicated in Eq. (20), we find that

$$L = \int_{cell} \cos (\underline{B} \cdot \underline{r}) \left[B_x J_{1x} + B_x J_{1y} \right] dV + \int_{cell} \sin (\underline{B} \cdot \underline{r}) \nabla \cdot \underline{J}_1 \, dV . \quad (21)$$

From Eqs. (13) and (14) we deduce that

$$j_{1,21} \equiv - \int \Omega_x I^{(0,1)} \, d\hat{\Omega} = 0 , \quad (22)$$

$$j_{1,12} \equiv - \int \Omega_y I^{(1,0)} \, d\hat{\Omega} = 0 . \quad (23)$$

Therefore,

$$J_{1x} = -B_x \int \Omega_x I^{(1,0)} \, d\hat{\Omega} \equiv B_x j_{1,11} , \quad (24)$$

$$J_{1y} = -B_y \int \Omega_y I^{(0,1)} \, d\hat{\Omega} \equiv B_y j_{1,22} . \quad (25)$$

Above, in Eqs. (22)-(25) we have made contact with Benoist's notation: the quantities $j_{1,k'k}$ have precisely the same meaning here as in Benoist's papers.[3] For those not familiar with Benoist's work we point out that the subscript 2 in the symbol $j_{1,21}$ indicates that the current

$j_{1,21}$ is produced by a source having Ω_y as a factor [see Eq. (13)]. The final subscript, 1, indicates that $j_{1,21}$ is a current in the x direction. Subscripts in the other quantities $j_{1,k'k}$ have similar meanings.

Since $\underline{J}_1$ is independent of y

$$\nabla \cdot \underline{J}_1 = B_x(\partial/\partial x)j_{1,11} \ . \tag{26}$$

Substituting from Eqs. (24), (25), and (26) into Eq. (21), we find that

$$L = \int_{cell} \cos \ (\underline{B} \cdot \underline{r}) \left[B_x^2 j_{1,11} + B_y^2 j_{1,22} \right] dV$$

$$+ B_x \int_{cell} \sin \ (\underline{B} \cdot \underline{r})(\partial/\partial x)j_{1,11} \ dV \ . \tag{27}$$

Let $\underline{r}_0$ be the midpoint of the cell, and assume (as we will in all our future work) that the cell is symmetric. Expanding L in a Taylor series in B_x and B_y, and retaining only leading terms, we find that

$$L = \cos \ (\underline{B} \cdot \underline{r}_0) \int_{cell} \left[B_x^2 j_{1,11} + B_y^2 j_{1,22} \right] dV$$

$$+ B_x \sin \ (\underline{B} \cdot \underline{r}_0) \int_{cell} (\partial/\partial x)j_{1,11} \ dV$$

$$+ B_x^2 \cos \ (\underline{B} \cdot \underline{r}_0) \int_{cell} (x - x_0)(\partial/\partial x)j_{1,11} \ dV$$

$$+ B_x B_y \cos \ (\underline{B} \cdot r_0) \int_{cell} (y - y_0)(\partial/\partial x)j_{1,11} \ dV \ . \tag{28}$$

Since $j_{1,11}$ is independent of y the last term on the right-hand side of Eq. (28) vanishes, and since $j_{1,11}$ is a periodic function of x, the second term also vanishes. Thus,

$$L = \cos(\underline{B} \cdot \underline{r}_0) \left\{ B_x^2 \left[\int_{cell} j_{1,11} \, dV + \int_{cell} (x - x_0)(\partial/\partial x) j_{1,11} \, dV \right] \right.$$

$$\left. + B_y^2 \int_{cell} j_{1,22} \, dV \right\} . \tag{29}$$

It should be noted that Eq. (29) is an exact expression for the leakage (in the limit B_x, $B_y \to 0$) if the series in B_x and B_y converges.

At this point Benoist asserts that effective diffusion constants must satisfy the relation

$$L = \left(D_x B_x^2 + D_y B_y^2 \right) \int_{cell} \phi(\underline{r}) \, dV , \tag{30}$$

where, as in Eq. (1)

$$\phi(\underline{r}) = \int F(\underline{r}, \hat{\Omega}) \, d\hat{\Omega} . \tag{31}$$

From Eq. (15) it is clear that

$$\phi(\underline{r}) = \cos(\underline{B} \cdot \underline{r}) \int R^{(0,0)} \, d\hat{\Omega} - \sin(\underline{B} \cdot \underline{r}) \int I_1 \, d\hat{\Omega} . \tag{32}$$

But I_1, as defined in Eq. (16), is first order in B. Therefore, neglecting higher-order terms,

$$\int_{cell} \phi(\underline{r}) \, dV = \cos(\underline{B} \cdot \underline{r}_0) \int_{cell} dV \int R^{(0,0)} \, d\hat{\Omega}$$

$$= \cos(\underline{B} \cdot \underline{r}_0) \int_{cell} \phi \, dV , \tag{33}$$

$$\phi \equiv \int d\hat{\Omega} \, R^{(0,0)} .$$

$$L = -\gamma \cos\left(\frac{\beta}{2} \cdot \gamma\right) \left\{ \frac{1}{2} \left[\int_{cell} \ldots dv - \int_{cell} \ldots dv \right] + \ldots \int_{cell} |\nabla \phi(\cos\beta)|^2 \ldots dv \right.$$

$$\left. + \frac{B}{2} \int_{cell} i',_{22} \, dv \right\}$$

It should be noted that Eq. (29) is an exact expression for the storage (in the limit B_x, $B_y \to 0$) if the series in B_x and B_y converge. At this point Reynolds asserts that effective diffusion constants may satisfy the relation

$$L = -\left(D_x B_x^2 + D_y B_y^2\right) \int_{cell} \phi(\underline{r}) \, dv ,$$

where, as in Eq. (1)

$$\phi(\underline{r}) = \int R(\underline{r}, t) \, dt .$$

From Eq. (18) it is clear that

$$\phi(\underline{r}) = \cos\beta \int_{cell} R^{(0,0)} \, dt - \sin\left(\frac{\beta}{2} \cdot \underline{r}\right) \int R^{(0,0)} I_1 \, dt$$

But I_1, as defined in Eq. (18), is first order in B. Therefore, neglecting higher-order terms,

$$\int \phi(\underline{r}) \, dv = \cos\beta \int_{cell} \, dv \int I_1 \left(\underline{r} - \underline{r}\right) R^{(0,0)} \, dt$$

$$= \cos\left(\frac{\beta}{2} \cdot \underline{r}\right) \int_{cell} \, dv \int$$

$$\int dt \, R^{(0,0)} .$$

Thus, to leading terms,

$$L = \left(D_x B_x^2 + D_y B_y^2\right) \cos \left(\underline{B} \cdot \underline{r}_0\right) \int_{cell} \phi(\underline{r}) \, dV \ . \tag{34}$$

Comparing Eq. (34) with Eq. (29) we conclude that

$$D_x \equiv D_1 = \left[\int_{cell} j_{1,11} \, dV + \int_{cell} (x - x_0)(\partial/\partial x)j_{1,11} \, dV\right] \Big/ \int_{cell} \phi \, dV \ , \tag{35}$$

$$D_y \equiv D_2 = \int_{cell} j_{1,22} \, dV \Big/ \int_{cell} \phi \, dV \ . \tag{36}$$

Given that

$$j_{1,k',k} = 0 \ , \qquad k' \neq k \tag{37}$$

from Eqs. (22) and (23), and that

$$(\partial/\partial y)j_{1,22} = 0 \tag{38}$$

from Eq. (26), one sees that Eqs. (35) and (36) are precisely, Benoist's equations for D_1 and D_2 specialized to a slab cell.[9]

Certainly it is possible to solve Eqs. (12), (13), and (14) in their present form (by discrete ordinate methods, for example) and to compute diffusion coefficients from Eqs. (35) and (36) directly. In the interests of efficiency, however, Benoist chooses to develop a computational procedure based on specially designed collision probability techniques. To facilitate the use of such techniques he introduces various approximations which we discuss next.

Thus, to leading terms,

$$L = \left\{ \left[D_x R_x^2 + D_y R_y^2 \right] \cos^2 (\underline{B} \cdot \underline{r}_x) \right\}_{cell} \cdot \phi(\underline{r}) \, dv \qquad (33)$$

Comparing Eq. (34) with Eq. (29) we conclude that

$$D_x = \overline{D}_x \cdot \left\{ \int_{cell} \overline{j}_{1,11} \, dv + \int_{cell} \left[(x - x_0)(\tau/\partial x)\overline{j}_{1,11} \right] dv \right\} \cdot dv \qquad (35)$$

$$D_y = \overline{D}_y \cdot \left\{ \int_{cell} \overline{j}_{1,22} \, dv \right\} \cdot dv \qquad (36)$$

Given that

$$\overline{j}_{1,x_i x_k} = 0, \qquad k \neq i \qquad (37)$$

from Eqs. (22) and (23), and that

$$[\partial/\partial x]\overline{j}_{1,xy} = 0 \qquad (38)$$

from Eq. (26), one sees that Eqs. (35) and (36) are precisely Benoist's
equations for D_x and D_y specialized to a slab cell.

Certainly it is possible to solve Eqs. (12), (13), and (14) in their
present form (by discrete ordinate methods, for example) and to compute
diffusion coefficients from Eqs. (35) and (36) directly. In the interest
of efficiency, however, Benoist chooses to develop a computational proce-
dure based on specially designed collision probability techniques. To
facilitate the use of such techniques he introduces various approxima-
tions which we discuss next.

It is easy to show that $I^{(0,1)}$, defined implicitly via Eq. (13), is proportional to Ω_y, i.e.

$$I^{(0,1)} = \Omega_y h(x,\mu) , \qquad \mu \frac{\partial h}{\partial x} + \Sigma_t h = -R^{(0,0)} , \qquad (39)$$

and it follows that the scattering term in Eq. (13) vanishes. We will assume, in Eqs. (13) and (14), that $R^{(0,0)}$ is almost isotropic, and replace $R^{(0,0)}$ with the scalar flux, ϕ. In this approximation we may write

$$\mu \frac{\partial \hat{h}}{\partial x} + \Sigma_t \hat{h} = -\phi , \qquad I^{(0,1)} \approx \hat{I}^{(0,1)} \equiv \Omega_y \hat{h} . \qquad (13')$$

Clearly, Eq. (13') can be solved without difficulty through the use of collision probabilities.

Now suppose that we set out to solve Eq. (14), as well, by collision probability methods, with $R^{(0,0)}$ replaced by ϕ. We see that the "uncollided flux," $I^{(1,0)}_{unc}$, produced by the source $\mu\phi$, is given by the expression

$$I^{(1,0)}_{unc} = \mu\hat{h} ,$$

where, again,

$$\mu \frac{\partial \hat{h}}{\partial x} + \Sigma_t \hat{h} = -\phi .$$

If we assume that $\hat{h}$ is isotropic, as is usual in collision probability calculations, then $I^{(1,0)}_{unc}$ is proportional to μ and the scattering integral again vanishes. Thus, the uncollided flux is the whole flux and we may write

$$\mu \frac{\partial \hat{h}}{x} + \Sigma_t \hat{h} = -\phi , \qquad I^{(0,1)} \approx \hat{I}^{(0,1)} \equiv \mu\hat{h} . \qquad (14')$$

It turns out that, if the scattering is not isotropic, and $\bar{\mu}$ is the mean cosine of the scattering angle, then

$$\mu \frac{\partial \hat{h}}{\partial x} + \Sigma_t \hat{h} = \frac{\bar{\mu}\Sigma_t}{4\pi} \int \hat{h} \, d\hat{\Omega} - \phi \, , \qquad I^{(1,0)} \approx \hat{I}^{(1,0)} \equiv \mu\hat{h} \, ;$$

but anisotropic scattering is a nonessential complication here and we shall continue to assume that the scattering is isotropic.

The numerator on the right-hand side of Eq. (35) contains two terms: the first is the volume integral of $j_{1,11}$, a quantity readily computed by collision probability methods. The computation of the second term is somewhat more difficult. One finds, however, that the second term is often small and the neglect of this term is generally considered to be part of what is called "Benoist's Method". In brief, then, Benoist's *approximate* diffusion constants are given by Eqs. (35') and (36'),

$$\hat{D}_1 = \int_{cell} \hat{j}_{1,11} \, dV \bigg/ \int_{cell} \phi \, dV \, , \qquad \hat{j}_{1,11} \equiv -\int \Omega_x \hat{I}^{(1,0)} \, d\hat{\Omega} \, , \quad (35')$$

$$\hat{D}_2 = \int_{cell} \hat{j}_{1,22} \, dV \bigg/ \int_{cell} \phi \, dV \, , \qquad \hat{j}_{1,22} \equiv -\int \Omega_y \hat{I}^{(0,1)} \, d\hat{\Omega} \, , \quad (36')$$

with $\hat{I}^{(1,0)}$ and $\hat{I}^{(0,1)}$ determined by Eqs. (13') and (14'), respectively.

On retracing the arguments that lead from Eq. (18) to Eq. (35), it will be seen that, to leading terms in the components of $\underline{B}$,

$$D_x \equiv D_1 = \int_{cell} (\partial/\partial x)\left(J_x\right) \, dV \bigg/ B_x^2 \int_{cell} \phi \, dV \, . \tag{40}$$

This expression for D_x follows directly from Eqs. (18) and (30). Undoubtedly Eq. (18) is a valid expression for the net leakage from the cell, but it is not clear how Benoist arrives at Eq. (30). In Benoist's published work

the relation is postulated without discussion. It is possible that Benoist considers that Eq. (30) is intuitively obvious: but, on the other hand, Bonalumi rejects this relation completely. Instead Bonalumi takes, as his definition of D_x, the expression

$$D_x(\text{BON}) = \int_{y_L}^{y_U} J_x\left(x_R, y\right) dy \Bigg/ \left\{ B_x \frac{\int_{y_L}^{y_U} \left[\phi\left(x_R, y\right) - \phi\left(x_L, y\right)\right] dy}{T} \right\}, \quad (41)$$

$$T = x_R - x_L .$$

Here y_U and y_L are, respectively, the y coordinates of the upper and lower cell boundaries. It is easy to show that in slab geometry the right-hand side of Eq. (41) will be independent of the values chosen for these coordinates. After trivial manipulation we find that

$$D_x(\text{BON}) = j_{1,11}\left(x_B\right) \Big/ \phi\left(x_B\right) , \quad (42)$$

where x_B is the x coordinate of either cell boundary.[10] In Eq. (42) we have used the notation $D_x(\text{BON})$ to make a sharp distinction between Bonalumi's D_x and the diffusion coefficients derived from Benoist's postulate, Eq. (30).

As was apparently first pointed out by Bonalumi,[4] Eq. (35), the equation defining Benoist's "exact" diffusion coefficient D_1, can be cast into a form quite similar to that of Eq. (42). After integrating over y in Eq. (35), then integrating by parts over x, we find that

$$D_1 = j_{1,11}\left(x_B\right) \Big/ \bar{\phi}_{\text{cell}} ,$$

$$\bar{\phi}_{\text{cell}} \equiv \int_{x_L}^{x_R} \phi(x) \, dx \Big/ T . \quad (43)$$

It will be seen that Eqs. (42) and (43) are identical except that in Eq. (42) the denominator is the cell-edge flux while in Eq. (43) it is the average flux. For this reason Bonalumi refers to his diffusion constant as "cell-edge normalized".

Perhaps it is fair to say that both Eqs. (40) and (41) seem perfectly plausible as definitions of the x diffusion coefficient. In arguing for the use of Eq. (41) in place of Eq. (40), Bonalumi asserts that the cell-edge normalized D_x (BON) satisfies Selengut's equivalence relation[11] while Benoist's D_1 does not, but this assertion is stated without proof. The relation between Benoist's and Bonalumi's x diffusion coefficient will be discussed further in later sections.

III. DOUBLE VALUE OF D_x

In Eqs. (42) and (43) various fluxes and currents are evaluated at the cell boundary. But in a symmetric cell there are two different sets of symmetry planes and correspondingly, *two* sets of cell boundaries (see Fig. 1). Thus there are two possible values of D_1, and of D_x (BON). It is easy to show that this ambiguity in the x diffusion coefficient is not *simply* due to a weakness in the definition but is inherent, in a sense, in the underlying physics. Suppose that $\Sigma(x)$ is the cross section for some arbitrarily chosen reaction in the lattice. Then the average reaction rate, $\bar{A}(x_0, B^2)$, within the cell is given by the expression

$$\bar{A}(x_0, B^2) = \int_{x_L}^{x_R} dx\ \Sigma(x) \int d\hat{\Omega}\ F(x,\hat{\Omega})/T , \tag{45}$$

$$\bar{A}(x_0, B^2) = (1/T) \int_{x_L}^{x_R} dx\ \Sigma(x) \left[\cos\left(B_x x\right) R(x,\hat{\Omega}) - \sin\left(B_x x\right) I(x,\hat{\Omega}) \right] d\hat{\Omega} . \tag{46}$$

Here we have arbitrarily set $y_0 = 0$; note that $\bar{A}(x_0,B^2)$ is a function of x_0 in the sense that it is the average reaction rate in a cell whose center is at x_0. Equation (46) is obtained by substituting from Eqs. (3) and (4) into Eq. (45). Now assume, for the sake of simplicity, that $B_y = 0$. One can then show from Eqs. (8) and (9) that $\psi(x) \equiv \int d\hat{\Omega}\, I(x,\mu)$ is antisymmetric in x about x_0. It follows that, to order B^2,

$$\bar{A}(x_0,B^2) = \frac{\cos(B\,x_0)}{T} \left\{ \int_{x_L}^{x_R} dx\, \Sigma(x)\rho(x) \right.$$

$$- \frac{1}{2} B^2 \int_{x_L}^{x_R} dx\, (x - x_0)^2 \Sigma(x)\psi(x)$$

$$\left. - B \int_{x_L}^{x_R} dx\, (x - x_0)\Sigma(x)\rho(x) \right\}. \tag{47}$$

Note that, since $\psi(x)$ is of order B, the last term in brackets is actually of order B^2, so that we may write

$$\bar{A}(x_0,B^2) = \frac{\cos(B\,x_0)}{T} \left[\int_{x_L}^{x_R} dx\, \Sigma(x)\rho(x) - c\, B^2 \right]. \tag{48}$$

Here, of course,

$$\rho(x) \equiv \int d\hat{\Omega}\, R(x,\mu)\,, \qquad \psi(x) \equiv \int d\hat{\Omega}\, I(x,\mu)\,, \tag{49}$$

and

$$c \equiv \frac{1}{2} \int_{x_L}^{x_R} dx (x - x_0)^2 \Sigma(x)\rho(x) + \int_{x_L}^{x_R} dx\, (x - x_0)\Sigma(x)\psi(x)\,. \tag{50}$$

Since Σ and ρ have the periodicity of the lattice, the integral in Eq. (48) is uniquely defined. On the other hand, it is clear from Eq. (50) that c can have either of two possible values, one for each of the two possible definitions of the unit cell.

Thus, the reaction rate (regarded as a function of x_0) has a cosine distribution over the lattice but there are two possible values one can assign to the amplitude of the cosine. Accordingly there will be two sets of "equivalent" homogenized cross sections which give reaction rates that match the cell-averaged reaction rates in the lattice. If the reaction rates and fluxes in the equivalent homogenized medium are to be correct at $B^2 = 0$, and if the effective cross sections are to be independent of buckling, then we must take

$$\bar{\Sigma} = \int_{x_L}^{x_R} \Sigma(x)\phi(x) \ dx/T \tag{51}$$

to be the homogenized reaction cross section. The two possible values of c then determine two diffusion constants, both equally acceptable.

When, as is customary, we neglect the second term in the numerator Eq. (35), then the diffusion coefficient is uniquely defined by Eq. (35'). It follows that, when such an approximation is valid, the difference between the two possible values of D_1 must be small. If, to the contrary, this second term is not negligible the spread between possible D_1 values may be significant. Usually $j_{1,11}$ will be positive for all x, and in such cases $\hat{D}_1$ will lie between these two possible values.

IV. NUMERICAL RESULTS

We propose, in this section: (1) to investigate the accuracy, in a typical ZPPR lattice, of the various approximations which are usually considered to be part of "Benoist's Method"; (2) to examine the differences in numerical values of D_x computed via cell-edge and cell-averaged normalization; and finally, to determine how large an uncertainty is introduced into D_x by the ambiguity in the definition of cell boundaries.

A. Diffusion Parallel to Plates

It turns out that cell-edge and cell-average normalization give the same expression for D_y, so that there is, in this case, no difference between the definitions proposed by Benoist and Bonalumi. Both lead us to Eq. (36). After carrying out the y integration in Eq. (36) we get

$$D_y = \int_{x_L}^{x_R} j_{1,22} \, dx \Big/ \int_{x_L}^{x_R} \phi \, dx . \tag{52}$$

Since D_y depends solely on integrals over the cell, and not on point values, it makes no difference which of the two alternative sets of symmetry planes we choose as cell boundaries: both choices give the same D_y. On the other hand, there is, of course, a difference between D_y and $\hat{D}_y$.

In a series of numerical experiments we have used the ANISN code[12] to compute the functions h and ĥ. This can be done, of course, in many ways, but we find it convenient to adopt the following procedure:

(1) We treat Eqs. (12) and (39) as the Group 1 and Group 2 equations, respectively, of a two-group set, with $\Sigma_{s\ell}^{1\to2} = -(2\ell + 1)/2$. Here $\Sigma_{s\ell}^{1\to2}$ is the $\ell'th$ Legendre component of the scattering cross section from Group 1 into Group 2.

(2) Equations (12) and (13') form another two-group set, but in this case $\Sigma_{s0}^{1 \to 2} = -(1/2)$, $\Sigma_{s\ell}^{1 \to 2} = 0$, $\ell > 0$. With h and $\hat{h}$ known, D_2 and $\hat{D}_2$ can be determined from Eqs. (36) and (36') respectively.

Coefficients D_2 and $\hat{D}_2$, for diffusion parallel to the plates, have been computed in this way for a typical ZPPR cell configuration. The cell geometry is sketched in Fig. 1, and all relevant problem parameters appear in Table I. Cross sections in this table are spectrum weighted over the range from 1 to 10 MeV but it is felt that details of the origin of these cross sections are not important here. We are interested only in an estimate of the accuracy of Benoist's diffusion coefficient rather than the exact value of this coefficient in some particular lattice.

To compute D_y we have solved Eqs. (12) and (39) in various S_n approximations characterized, in Table II, as DP_3-P_7, DP_4-P_9, and DP_5-P_{11}. Here the designation DP_5-P_{11} refers to an S_n approximation with

(1) 12 double-Gauss quadrature weights and ordinates, appropriate to a double-P_5 approximation; and

(2) delta-function scattering from Group 1 into Group 2, represented in a P_{11} approximation.

The other designations have corresponding interpretations. In the computation of $\hat{D}_2$, Eqs. (12) and (13') were again solved in DP_3, DP_4, and DP_5 approximations, but with anisotropic scattering from Group 1 into Group 2 suppressed, as indicated in the lower rows of Table II. It is very clear from Table II that Benoist's method, which yields $\hat{D}_2$ instead of D_2, is extremely accurate in this case despite the strong anisotropy of the angular flux.

B. Diffusion Normal to Plates

Making use of the knowledge that $I^{(0,1)}$ is proportional to Ω_y, it is possible, as we have seen, to compute this quantity by solving Eq. (39) on standard S_n codes. Similarly standard S_n codes can be used to solve Eq. (13') for $\hat{h}$ which, then, gives us both $\hat{I}^{(0,1)}$ and $\hat{I}^{(1,0)}$. The computation of $I^{(1,0)}$ is slightly more difficult.

The quantity $I^{(1,0)}$ is determined by Eq. (14), which differs from the usual neutron transport equation in two respects. First, the coupling term, $\mu R^{(0,0)}$ cannot be developed in a Legendre polynomial expansion of the required form, i.e.,

$$\mu R^{(0,0)} \neq \sum_{\ell=0}^{\infty} \left(\frac{2\ell + 1}{2} \right) \Sigma_{s\ell} R_\ell^{(0,0)} P_\ell(\mu)$$

for any set of numbers $\Sigma_{s\ell}$. Secondly, one can show that

$$I^{(1,0)}(x,\mu) = -I^{(1,0)}(x,-\mu) , \qquad x = x_L \text{ or } x = x_R . \tag{53}$$

Equation (53) defines a boundary condition ("antisymmetry condition") which is not available in standard S_n codes. On the other hand, it is not difficult to write a two-group S_n code which permits the imposition of "antisymmetric" boundary conditions and, in addition, includes the term $\mu R^{(0,0)}$ as a source into the second group. Such a code has been written, and used to solve Eqs. (12) and (14).

Essentially three different approximations are involved in the process which takes us from D_1 to $\hat{D}_1$. First, one neglects the second term in the numerator of Eq. (35): second, one replaces the source term $\mu R^{(0,0)}$ with the source term $\mu\phi$: finally, the scattering term in Eq. (14) is deleted. Since the angular flux in the test problem

configuration is highly anisotropic, it is interesting to ask how much error is introduced into the effective diffusion coefficient by the second step alone.

Suppose that, in Eq. (14), we replace $\mu R^{(0,0)}$ by $\mu\phi$ without making any other changes. Define a function $\bar{I}^{(1,0)}$ such that

$$\mu \frac{\partial \bar{I}^{(1,0)}}{\partial x} + \Sigma_t \bar{I}^{(1,0)} = \frac{\Sigma_s}{4\pi} \int d\hat{\Omega} \ \bar{I}^{(1,0)} - \mu\phi \ . \tag{14"}$$

Let

$$\bar{j}_{1,11} = -\int \hat{\Omega} \ d\hat{\Omega} \ \bar{I}^{(1,0)} \ ,$$

and

$$\bar{D}_1 = \int_{x_L}^{x_R} \bar{j}_{1,11} \ dx \Big/ \int_{x_L}^{x_R} \phi \ dx \ , \tag{35"}$$

while

$$\bar{\bar{D}}_1 \equiv \int_{x_L}^{x_R} j_{1,11} \ dx \Big/ \int_{x_L}^{x_R} \phi \ dx \ . \tag{35'''}$$

We see that the difference between $\bar{D}_1$ and $\bar{\bar{D}}_1$ reflects only the effect of anisotropy in $R^{(0,0)}$.[13]

Values of $\bar{D}_1$ and $\bar{\bar{D}}_1$, computed in various S_n approximations, are listed in Table III. It will be seen that the anisotropy in the source term has no appreciable influence on the integral of the effective current $j_{1,11}$. It seems remarkable that this should be true, in view of the fact that the flux, $R^{(0,0)}$, is so strongly anisotropic.

configuration is phenomenological... it is interesting to ask how much error is introduced into the effective diffusion coefficient by the second step alone.

Suppose that, in Eq. (14), we replace $R_{ik}^{(0,0)}$ by R_0 as without making any prior change. Define a function $\bar{f}_{ij}(0,0)$ such that

$$\frac{\bar{f}_{ij}(0,0)}{...} = ... \bar{a}_{ij}(0,0) ... a_{ij}(0,0) ... \qquad [34']$$

$$\bar{f}_{ij}(0,0) = ... a_{ij}(0,0) \qquad [35']$$

and

$$\bar{g}_{ij} = ... \int_{...}^{...} ... dx_i \int_{...}^{...} ... dx_j , \qquad [35']$$

while

$$\bar{B}_{ij} = ... \int_{...}^{...} dx_i \int_{...}^{...} ... dx_j . \qquad [36'']$$

We see that the difference between $\bar{g}_{ij}$ and $\bar{B}_{ij}$ reflects only the effect of attraction in $\bar{f}_{ij}(0,0)$, be...

... values of $\bar{g}_{ij}$ and $\bar{B}_{ij}$ computed in various $\bar{f}_{ij}$ approximations, are listed in Table III. It will be seen that the anisotropy in the source term has no appreciable influence on the integral of the effective current $\bar{g}_{ij}$. It seems remarkable that this should be true, in view of the fact that the function $R_{ij}^{(0,0)}$ is so strongly anisotropic.

In Table IV we list values of D_x computed according to various prescriptions. Diffusion coefficients which appear in the first row of numbers are computed from the Benoist definitions: $D_1^A(x_B)$ and $D_1^B(x_B)$ are "exact" Benoist diffusion coefficients, defined in Eq. (43), while $\hat{D}_1$ is the "approximate" Benoist diffusion coefficient defined via Eq. (35'). It is this last diffusion coefficient which one would refer to, customarily, as the diffusion coefficient given by Benoist's method. We see that $D_1^A(x_B)$ and $D_1^B(x_B)$ differ by about 2%. On the other hand, since $\hat{D}_2 \simeq 2.88$ (see Table II), $\hat{D}_1$ and $\hat{D}_2$ differ by about 4%. Thus, the magnitude of the anisotropic effect is uncertain by 50%.

If, in Eq. (14) we simply replace the coupling term, $\mu R^{(0,0)}$, by the approximate coupling term $\mu\phi$, as in Eq. (14"), we get $\bar{I}^{(1,0)}$ in place of $I^{(1,0)}$. Suppose that we use the currents $\bar{j}_{1,11}(x_B)$ to define diffusion coefficients in place of the "exact" current $j_{1,11}(x_B)$. Diffusion coefficients so defined are listed in the second row of numbers in Table IV. As one might expect, the anisotropy of the flux has a much greater effect on the value of $j_{1,11}$ at individual points than it has on the volume integral of $j_{1,11}$. In fact the use of the scalar flux instead of the angular flux cuts in half the spread between the two permissible diffusion coefficients.

It turns out that the scalar flux, ϕ, varies much more over the test problem configuration, than does the effective current $j_{1,11}$. As a result the two cell-edge normalized diffusion coefficients, which appear in the last row of Table IV, are much farther apart than the corresponding coefficients as defined by Benoist. Moreover, they are much farther apart than the Benoist x and y diffusion coefficients, $\hat{D}_1$ and $\hat{D}_2$. Thus, the spread between permissible values of the Bonalumi x diffusion coefficient totally obscures any anisotropic diffusion effect in the ZPPR lattice.

V. CRITERIA FOR THE VALIDITY OF THE HOMOGENIZATION PROCESS

We see that there are substantial differences between the x diffu-
sion coefficients as defined by Benoist and Bonalumi. Certainly we are
left in an awkward position if we accept Bonalumi's definition, since the
spread in permissible x diffusion coefficients is, then, so large. It
does not follow, however, that Bonalumi's definition is wrong, or that
Benoist's definition is right. In fact we have, at this point, adopted
no criterion by which to judge either definition.

It is true that Selengut's equivalence principle[11] leads unambiguously
to a definition of effective diffusion coefficients *in certain circumstances*.
Selengut assumes, in Ref. 11, that diffusion theory is valid and that the
absorption cross section vanishes. The direct application of Selengut's
principle under more general conditions is not an entirely straightforward
extension of his work and we prefer, here, to explore other approaches.

A. Assessment of the Performance of Homogenized Diffusion Coefficients

Consider, again, the one-energy transport equation, Eq. (1), and
assume for simplicity that $B_y = 0$. Given a lattice cell with boundaries
at x_L and x_R, define

$$\bar{\Phi}_{HET} = \int_{x_L}^{x_R} \Phi_{HET}(x) \, dx/T \ . \tag{54}$$

Here $\Phi_{HET}(x)$ is the scalar flux in the heterogeneous assembly and $T = x_R - x_L$.
It is clear that

$$\bar{\Phi}_{HET} = \bar{Q}/\left[\Sigma_a + D_1 B^2\right] \ , \tag{55}$$

where

$$\bar{Q} = \int_{x_L}^{x_R} q(x) \cos (Bx) \, dx/T \; , \tag{56}$$

$$\bar{\Sigma}_a = \int_{x_L}^{x_R} \phi(x)\Sigma_a(x) \, dx \bigg/ \int_{x_L}^{x_R} \phi(x) \, dx \; , \tag{57}$$

$$D_1 = \int_{x_L}^{x_R} (\partial/\partial x) \, J_x \, dx \bigg/ \int_{x_L}^{x_R} \phi(x) \, dx \; . \tag{58}$$

It will be seen, on comparison with Eq. (40), that D_1 is precisely the x diffusion coefficient as defined by Benoist, but it should be noted that $\bar{Q}$ and $\bar{\Sigma}_a$ are functions of the buckling. To order B^2

$$\bar{Q} = Q^{(0)} + Q^{(2)}B^2 \; , \qquad Q^{(0)} = \bar{q} \cos (Bx_0) \; , \qquad \bar{q} \equiv \int_{x_L}^{x_R} q(x) \, dx/T \; , \tag{59}$$

and

$$\bar{\Sigma}_a = \Sigma_a^{(0)} + \Sigma_a^{(2)}B^2 \; , \qquad \Sigma_a^{(0)} = \int_{x_L}^{x_R} \phi(x)\Sigma_a(x) \, dx \bigg/ \int_{x_L}^{x_R} \phi(x) \, dx \; . \tag{60}$$

Thus we may write

$$\bar{\phi}_{HET} = \frac{\left[Q^{(0)} + Q^{(2)}B^2 \right]}{\left[\Sigma_a^{(0)} + \left[\Sigma_a^{(2)} + D_1 \right]B^2 \right]} \; . \tag{61}$$

In the homogenized assembly one generally takes, as the effective absorption cross section, the quantity

$$\left(\Sigma_a \right)_{HOM} = \int_{x_L}^{x_R} \phi(x)\Sigma_a(x) \, dx \bigg/ \int_{x_L}^{x_R} \phi(x) \, dx$$

$$= \Sigma_a^{(0)} \; , \tag{62}$$

while the source density is given by the expression

$$Q_{HOM} = \bar{q} \cos (Bx) . \tag{63}$$

Expanding in powers of B and averaging over the cell we find that

$$\bar{Q}_{HOM} = Q^{(0)} - (1/24)B^2 T^2 \bar{q} \cos (Bx_0) ,$$

$$= Q^{(0)} - (1/24)T^2 B^2 Q^{(0)} . \tag{64}$$

Thus, given a homogenized x diffusion coefficient D_x,

$$\bar{\Phi}_{HOM} = \frac{\left[Q^{(0)} - (1/24)T^2 B^2 Q^{(0)} \right]}{\left[\Sigma_a^{(0)} + D_x B^2 \right]} . \tag{65}$$

If $\Delta \equiv Q^{(2)} - (1/24) T^2 Q^{(0)}$, then

$$\bar{\Phi}_{HOM} = \frac{\left[Q^{(0)} + Q^{(2)} B^2 - B^2 \Delta \right]}{\left[\Sigma_a^{(0)} + D_x B^2 \right]} , \tag{66}$$

so that, to order B^2,

$$\bar{\Phi}_{HOM} = \frac{\left[Q^{(0)} + Q^{(2)} B^2 \right]}{\Sigma_a^{(0)} + \left[D_x + \Sigma_a^{(0)} \left(\Delta/Q^{(0)} \right) \right]} . \tag{67}$$

From Eqs. (61) and (67) it is clear that $\bar{\Phi}_{HOM}$ and $\bar{\Phi}_{HET}$ will be different unless

$$D_x = D_1 + \Sigma_a^{(2)} - \Sigma_a^{(0)} \left(\Delta/Q^{(0)} \right) . \tag{68}$$

We see that if the effective absorption cross section and the source are defined as in Eqs. (62) and (63) respectively, then both the Bonalumi and Benoist prescriptions will yield incorrect average fluxes within the

boundaries of each cell. Further, even if we were to use Eq. (68) to define an effective diffusion coefficient (again double-valued), the absorption rate, AR, in the cell would be given, to order B^2, by the expression

$$AR = \left[\Sigma_a^{(0)} + \Sigma_a^{(2)} B^2 \right] \bar{\Phi}_{HOM} T , \tag{69}$$

and

$$AR \neq \Sigma_a^{(0)} \bar{\Phi}_{HOM} T .$$

We do not mean to suggest, at this point, that a prescription involving a buckling-dependent absorption cross section would actually be practical. Rather it is our intention to point out that the defects in present homogenization schemes will not be easy to remedy.

When $B_x = 0$, $B_y \neq 0$, we again find, by similar arguments, that the Benoist method gives an incorrect average flux in the interval which corresponds to the extent of any cell. In this case, however, it turns out, when one uses Benoist's D_2 as the diffusion coefficient, that $\Sigma_a^{(0)} \bar{\Phi}_{HOM}(\underline{r}_0)$ is the correct average absorption rate in the cell centered at $\underline{r}_0$. Again we recall that the Benoist and Bonalumi D_y are the same.

It seems important to be aware of these deficiencies in the Bonalumi and Benoist methods, deficiencies which we have noted in the Bonalumi and Benoist treatments of the inhomogeneous transport equation. But it is not necessarily true that one should go so far as to redefine diffusion coefficients with the inhogeneous transport equation specifically in mind. In fact it may be better, at this point, to turn our attention from inhomogenous to eigenvalue problems.

B. **Reformulation of Definition of Effective Diffusion Coefficients**

In our notation the one-group transport equation with fission and isotropic scattering takes the form

$$\mu(\partial R/\partial x) + \Sigma_t R = \left(\Sigma_s/4\pi\right)\phi + (1/\lambda)\left(\nu\Sigma_f/4\pi\right)\phi + (\hat{\Omega} \cdot \underline{B})I , \tag{70}$$

$$\mu(\partial I/\partial x) + \Sigma_t I = \left(\Sigma_s/4\pi\right)\psi + (1/\lambda)\left(\nu\Sigma_f/4\pi\right)\psi - (\hat{\Omega} \cdot \underline{B})R , \tag{71}$$

where

$$\phi \equiv \int R \, d\hat{\Omega} \tag{72}$$

and

$$\psi \equiv \int I \, d\hat{\Omega} . \tag{73}$$

Suppose we consider the term $(\hat{\Omega} \cdot \underline{B})I$ in Eq. (70) as a perturbation, defining "unperturbed" eigenvalue equations as follows:

$$\mu(\partial\tilde{R}/\partial x) + \Sigma_t\tilde{R} = \left(\Sigma_s/4\pi\right)\tilde{\phi} + (1/\lambda_0)\left(\nu\Sigma_f/4\pi\right)\tilde{\phi} , \tag{74}$$

$$\mu(\partial\tilde{I}/\partial x) + \Sigma_t\tilde{I} = \left(\Sigma_s/4\pi\right)\tilde{\psi} + (1/\lambda_0)\left(\nu\Sigma_f/4\pi\right)\tilde{\psi} - (\hat{\Omega} \cdot \underline{B})\tilde{R} . \tag{75}$$

It will be seen that each unperturbed eigenvalue, λ_0, is actually degenerate with eigenvectors

$$\underline{V}_1 = \begin{pmatrix} \tilde{R} \\ \tilde{I} \end{pmatrix} , \qquad \underline{V}_2 = \begin{pmatrix} 0 \\ \tilde{R} \end{pmatrix} . \tag{76}$$

The unperturbed adjoint equations appear below:

$$-\mu(\partial\tilde{R}^*/\partial x) + \Sigma_t\tilde{R}^* = \left(\Sigma_s/4\pi\right)\tilde{\phi}^* + (1/\lambda_0)\left(\nu\Sigma_f/4\pi\right)\tilde{\phi}^* - (\tilde{\Omega} \cdot \underline{B})\tilde{I}^* \quad,(77)$$

$$-\mu(\partial\tilde{I}^*/\partial x) + \Sigma_t\tilde{I}^* = \left(\Sigma_s/4\pi\right)\tilde{\psi}^* + (1/\lambda_0)\left(\nu\Sigma_f/4\pi\right)\tilde{\psi}^* \quad, \tag{78}$$

Again, for each λ_0 there are two eigenvectors which we may write as follows:

$$\underline{V}_1^* = \begin{bmatrix} \tilde{R}(-\mu) \\ 0 \end{bmatrix}, \qquad \underline{V}_2^* = \begin{bmatrix} -\tilde{I}(-\hat{\Omega}) \\ \tilde{R}(-\mu) \end{bmatrix} . \tag{79}$$

Let

$$\Delta H = \begin{bmatrix} 0 & -(\hat{\Omega} \cdot \underline{B}) \\ 0 & 0 \end{bmatrix} .$$

It is easy to see that

$$\left\langle \underline{V}_1^\dagger \underline{V}_j \right\rangle = 0 \;, \qquad i \neq j \;, \tag{80}$$

$$\left\langle \underline{V}_i^*(\Delta H)\underline{V}_j \right\rangle = 0 \;, \qquad i \neq j \;. \tag{81}$$

Here

$$\left\langle UV \right\rangle \equiv \int d\hat{\Omega} \int_{x_L}^{x_R} U(x,\hat{\Omega})V(x,\hat{\Omega}) \; dx \;.$$

Further one can show that

$$\left\langle \underline{V}_1^*(\Delta H)\underline{V}_1 \right\rangle = \left\langle \underline{V}_2^*(\Delta H)\underline{V}_2 \right\rangle \;,$$

$$\left\langle \underline{V}_1^*\left(\nu\Sigma_f I\right)\underline{V}_1 \right\rangle = \left\langle \underline{V}_2^*\left(\nu\Sigma_f I\right)\underline{V}_2 \right\rangle \;,$$

where I is the identity operator. Therefore it follows from degenerate perturbation theory that there is only one perturbed eigenvalue, given by the expression

$$(1/\lambda) = (1/\lambda_0) + \left\langle \underline{V}_1^*(\Delta H)\underline{V}_1 \right\rangle \Big/ \left\langle \underline{V}_1^*\left(\nu\Sigma_f I\right)\underline{V}_1 \right\rangle . \tag{82}$$

More explicitly

$$(1/\lambda) = (1/\lambda_0) - \int d\Omega \int_{x_L}^{x_R} \tilde{R}(-\mu)(\hat{\Omega} \cdot \underline{B})\tilde{I}(\hat{\Omega}) \, dx/F . \tag{83}$$

Here

$$F \equiv \int_{x_L}^{x_R} \left(\nu\Sigma_f\right)\tilde{\phi}^2 \, dx .$$

Define $\tilde{I}_x$ and $\tilde{I}_y$ such that

$$\mu\left(\partial\tilde{I}_x/\partial x\right) + \Sigma_t\tilde{I}_x = \left(\Sigma_s/4\pi\right)\tilde{\psi} + (1/\lambda_0)\left(\nu\Sigma_f/4\pi\right)\tilde{\psi} - \mu B_x\tilde{R} , \tag{84}$$

$$\mu\left(\tilde{I}_y/\partial y\right) + \Sigma_t\tilde{I}_y = -\Omega_y B_y\tilde{R} , \tag{85}$$

$$\tilde{\psi} \equiv \int d\hat{\Omega} \, \tilde{I}_x .$$

It can easily be shown that Eqs. (84) and (85) do have solutions, despite the fact that $(1/\lambda_0)$ is an eigenvalue of the corresponding homogeneous equations. Further $\tilde{I} = \tilde{I}_x + \tilde{I}_y$ and, finally,

$$-\int d\hat{\Omega} \int_{x_L}^{x_R} \tilde{R}(-\mu)(\hat{\Omega} \cdot \underline{B})\tilde{I}(\hat{\Omega}) \, dx = B_x^2\tau_x + B_y^2\tau_y , \tag{86}$$

where

$$\tau_x \equiv -\int d\hat{\Omega} \int_{x_L}^{x_R} \mu R(-\mu)\tilde{I}_x(\mu) \, dx/F ,$$

$$\tau_y \equiv -\int d\hat{\Omega} \int_{x_L}^{x_R} \Omega_y\tilde{R}(-\mu)\tilde{I}_y(\hat{\Omega}) \, dx/F .$$

From Eqs. (83) amd (86) it follows that

$$(1/\lambda) = (1/\lambda_0) + B_x^2\tau_x + B_y^2\tau_y . \tag{87}$$

Now

$$\lambda_0 = \overline{\nu\Sigma_f}^{(0)}\Big/\overline{\Sigma_a}^{(0)} , \tag{88}$$

where

$$\overline{\nu\Sigma_f}^{(0)} \equiv \int_{x_L}^{x_R} \left(\nu\Sigma_f\right)\tilde{\phi}(x)\, dx \Big/ \int_{x_L}^{x_R} \tilde{\phi}(x)\, dx , \tag{89}$$

$$\overline{\Sigma}^{(0)} = \int_{x_L}^{x_R} \Sigma_a\tilde{\phi}(x)\, dx \Big/ \int_{x_L}^{x_R} \tilde{\phi}(x)\, dx . \tag{90}$$

Therefore we may write Eq. (87) in the form

$$(1/\lambda) = \left[\overline{\Sigma}_a^{(0)}\Big/\overline{\nu\Sigma_f}^{(0)}\right]\left\{1 + \left[\overline{\nu\Sigma_f}^{(0)}\Big/\overline{\Sigma}_a^{(0)}\right]\left(\tau_x B_x^2 + \tau_y B_y^2\right)\right\} ,$$

$$= \left\{\overline{\Sigma}_a^{(0)} + \left[\overline{\nu\Sigma_f}^{(0)}\right]\tau_x B_x^2 + \left[\overline{\nu\Sigma_f}^{(0)}\right]\tau_y B_y^2\right\}\Big/\overline{\nu\Sigma_f}^{(0)} . \tag{91}$$

It will be seen from Eq. (91) that, if we take $\overline{\Sigma}^{(0)}$ and $\overline{\nu\Sigma_f}^{(0)}$ as the "equivalent homogenized" Σ_a and $\nu\Sigma_f$, respectively, then $\left[\overline{\nu\Sigma_f}^{(0)}\right]\tau_x$ plays the role of D_x, while $\left[\overline{\nu\Sigma_f}^{(0)}\right]\tau_y$ plays the role of D_y. We are led, then, to define

$$D_x^{(\lambda)} = \left[-\int d\hat{\Omega}\int_{x_L}^{x_R} \mu\tilde{R}(-\mu)\tilde{I}_x(\mu)\, dx\right]\int_{x_L}^{x_R} \left(\nu\Sigma_f\right)\tilde{\phi}(x)\, dx \Big/ \int_{x_L}^{x_R} \left(\nu\Sigma_f\right)\tilde{\phi}^2(x)\, dx , \tag{92}$$

$$D_y^{(\lambda)} = \left[-\int d\hat{\Omega}\int_{x_L}^{x_R} \Omega_y\tilde{R}(-\mu)\tilde{I}_y(\hat{\Omega})\, dx\right]\int_{x_L}^{x_R} \left(\nu\Sigma_f\right)\tilde{\phi}(x)\, dx \Big/ \int_{x_L}^{x_R} \left(\nu\Sigma_f\right)\tilde{\phi}^2(x)\, dx . \tag{93}$$

Suppose that, in Eq. (82), we approximate the importance function, $\underline{V}_1^*$, by its average over space and solid angle. We find, in this approxima-

$$D_x^{(\lambda)} \approx \int_{x_L}^{x_R} \tilde{j}_{1,11} \, dx \bigg/ \int_{x_L}^{x_R} \tilde{\phi}(x) \, dx \;, \tag{94}$$

and,

$$D_y^{(\lambda)} \approx \int_{x_L}^{x_R} \tilde{j}_{1,22} \, dx \bigg/ \int_{x_L}^{x_R} \tilde{\phi}(x) \, dx \;. \tag{95}$$

Further, if we now compute $\tilde{j}_{1,11}$ and $\tilde{j}_{1,22}$ by Benoist's collision probability methods, $D_x^{(\lambda)}$ and $D_y^{(\lambda)}$ become, identically, Benoist's $\hat{D}_1$ and $\hat{D}_2$. Thus there is a close connection between Benoist's diffusion coefficients and the diffusion coefficients required to preserve the eigenvalue during homogenization. Perhaps this close connection gives us a justification of some sort for the use of Benoist's method: at the moment we see no similar justification for the use of Bonalumi's method.

We digress here to note that the effective diffusion coefficients defined in Eqs. (92) and (94) differ from those derived earlier by Williams.[14] On comparing Eq. (77) in Ref. 14 with our Eq. (40), one finds that Williams' x diffusion coefficient, $\bar{D}_x$, is identical with the Benoist D_1. Williams apparently concludes that the diffusion coefficient $\bar{D}_x$ (or D_1), used in conjunction with $\bar{\Sigma}_a^{(0)}$ and $\overline{\nu\Sigma_f}^{(0)}$, reproduces the heterogeneous lattice eigenvalue. Yet it would seem that this cannot be true, simply because D_1 is double-valued if for no other reason.

It is difficult to compare Williams' work, in detail, with our own since the mathematical techniques used here and in Ref. 14 are, formally, quite different. We believe, however, that the discrepancies between our results and those reported by Williams can be traced back to a fundamental assumption embodied in Eq. (3) of Ref. 14. Williams postulates that $k_{eff} = k_\infty P$, where P is the nonleakage probability. We have argued, above,

that k_{eff} and k_∞ differ, not only because of the direct effect of leakage, but also because (to order B^2) the leakage modifies the effective absorption and fission cross sections. We see no treatment of such indirect effects in Williams' derivation.

Diffusion coefficients defined by Eqs. (92) and (93) have not yet been computed for our ZPPR test problem configuration. It is possible, however, to make a rough estimate of the ratios between these coefficients, on the one hand, and Benoist's on the other. We have already seen that approximations based on the assumption that R is isotropic tend to be very accurate. It has also been noted earlier that $j_{1,11}$ is nearly constant over the ZPPR cell and, in fact, we observe that $j_{1,22}$ is also nearly constant. If it is assumed that R is isotropic, and that both $j_{1,11}$ and $j_{1,22}$ are constant, we find that

$$\left[D_x^{(\lambda)}/\hat{D}_1 \right] \approx \left[\int_{x_L}^{x_R} \left(\nu\Sigma_f \right) \bar{\phi}\, dx \middle/ \int_{x_L}^{x_R} \left(\nu\Sigma_f \right) \bar{\phi}^2\, dx \right] \left[\int_{x_L}^{x_R} \bar{\phi}\, dx \middle/ T \right]$$

$$\approx \left[D_y^{(\lambda)}/\hat{D}_2 \right] . \tag{96}$$

In order to make an estimate of the value of the integrals on the right-hand side of Eq. (96), we assume, further, that $\bar{\phi}$ is approximately equal to the scalar flux, ϕ, computed earlier, in our fixed-source test problem. It will be recalled that, in this fixed source problem, the source in each region was taken to be equal to $\nu\Sigma_f$ in that region. It seems not unreasonable, therefore, to assume that ϕ and $\bar{\phi}$ have roughly the same shape. At any rate if we make this assumption we come to the conclusion that

$$\left[D_x^{(\lambda)} / \hat{D}_1 \right] \; \underset{\sim}{\sim} \; \left[D_y^{(\lambda)} / \hat{D}_2 \right] \; \underset{\sim}{\sim} \; 0.964 \; , \tag{97}$$

i.e. that Benoist's D's are too small, in this case, by about three to four percent.

We believe that Eqs. (92) and (93) can be generalized straightforwardly to the multigroup case, at least in situations where the group-to-group scattering is taken to be isotropic. Generalized versions of these equations could be used to test Benoist's method, or to correct Benoist's diffusion coefficients when corrections are deemed necessary. It should be stressed, at this point, that the proposed new definitions of D_x and D_y are contrived for one purpose alone: they are designed to reproduce, in the homogenized lattice, the eigenvalue of the heterogeneous lattice. The eigenvalue in the homogenized lattice will be correct to order B^2 if the new diffusion coefficients are used in conjunction with the buckling-independent one-group parameters defined in Eqs. (89) and (90). On the other hand, edited reaction rates (for any given power level) will not be correct to order B^2 unless the reaction cross sections are *buckling dependent;* and, unfortunately it is not clear that the use of buckling-dependent reaction cross sections would actually be feasible in the analysis of real reactors. Thus the new prescription for the computation of diffusion coefficients shares some of the weaknesses of older prescriptions.

How important these weaknesses are, from a practical point of view, we cannot say. Further it should be pointed out that very little is known, at this time, about the performance of any homogenization scheme near interfaces. In view of the difficulty of a more thorough theoretical analysis

it seems clear that, ultimately, only detailed Monte Carlo calculations can give us the information we need for definitive tests of our and other homogenization procedures.

VII. CONCLUSIONS

In the particular version of the ZPPR which we have studied here the probability of leakage out of the core is, approximately, 30%, and the leakage probabilities in the x, y, and z directions are roughly equal. Further the Benoist x diffusion coefficient, $\hat{D}_1$, turns out to be almost equal to the diffusion coefficient, $\bar{D}$, computed from the flux-weighted transport cross section. On the other hand, the y and z Benoist diffusion coefficients, $\hat{D}_2$ and $\hat{D}_3$, are greater than $\bar{D}$ by about 4%. It follows that when we use the Benoist method, taking $\hat{D}_1$, $\hat{D}_2$, and $\hat{D}_3$ (in place of $\bar{D}$) for the x, y, and z diffusion coefficients, we lower the eigenvalue, k_{eff}, by about 0.8%. If, now, we assume that D_1 is uncertain by 2%, an amount corresponding to the spread between the two permissible values of D_1, we conclude that k_{eff} is uncertain by roughly 0.2%. Such an uncertainty is not particularly significant, and is fairly small compared to the 0.8% change in k_{eff} caused, in toto (according to Benoist's method), by aniso-tropic diffusion. In contrast the 11% spread in Bonalumi's x diffusion coefficient gives rise to a 1% uncertainty in eigenvalue, an uncertainty which is significant, and is no smaller than the whole anisotropy effect. Moreover Bonalumi's definition of effective diffusion coefficients seems as appealing, intuitively, as Benoist's.

Since intuition does not seem to lead us to one unique definition of D_1, we have found it necessary to formulate a precise objective of some

sort for the homogenization process. The objective we have chosen is quite simple. We wish to construct buckling independent group parameters such that the homogeneous eigenvalue (i.e. the eigenvalue in the homogenized lattice) will be equal to the heterogeneous eigenvalue to order B^2. Suitable parameters are defined, for one-group problems, in Section V. It seems clear that corresponding multigroup parameters can be obtained by straightforward generalization of the methods of Section V if the P_1 transfer matrix is diagonal.

The diffusion coefficients defined in Section V are ratios of integrals whose integrands contain importance functions. If we approximate these importance functions by their average values we find that our $D_x^{(\lambda)}$ and $D_y^{(\lambda)}$ become identically the same as Benoist's $\hat{D}_1$ and $\hat{D}_2$, respectively. This close connection between $\hat{D}$ and the diffusion coefficients required to preserve k_{eff} seems to provide some measure of justification for the use of Benoist's method.

It is interesting to note, however, that if one advocates the use of Benoist's method on such grounds one cannot, any longer, consider the term

$$\Delta D_1 \equiv \int_{x_L}^{x_R} (x - x_0)\left(\partial j_{1,11}\Big/\partial x\right) dx \Bigg/ \int_{x_L}^{x_R} \phi \, dx$$

as a correction to $\hat{D}_1$. The quantity $\hat{D}_1$ will generally lie somewhere within the interval bounded by the two values of D_1. By adding ΔD_1 to $\hat{D}_1$ one moves the x diffusion coefficient, from some point inside this interval, to a new point close to one of its boundaries. But it is difficult to see why either boundary value, $D_1\left(x_B\right)$, should be any more correct than $\hat{D}_1$.

If we take $D_x^{(\lambda)}$ and $D_y^{(\lambda)}$ to be the "true" homogenized diffusion coefficients there does not seem to be any simple expression for the errors in $\hat{D}_1$ and $\hat{D}_2$. In Section V we have tried to estimate the magnitude of these errors in our test problem and have concluded that $\hat{D}_1$ and $\hat{D}_2$ are too large by about 3.4%. Such errors in Benoist's D's would produce a 1% error in k_{eff} in the reactor configuration under consideration here. Now, our test problem is a one-group problem with group parameters covering the range from 1 to 10 MeV. In a multigroup adjoint computation the group in question would contain "slowing-down" sources coupling it to groups of lower energies. Because of the absence of such fictitious slowing-down sources in the one-group adjoint equations it is possible that the one-group and multigroup importance functions will be quite different in shape. Therefore one cannot assume that our estimate of the errors in Benoist's D's will be very accurate. Nevertheless our results do seem to indicate that these errors may be significant and should be examined further.

Many weaknesses in the treatment of anisotropic diffusion remain. The group parameters which enter into eigenvalue calculations would, according to our proposal, be buckling independent. But if we are to compute reaction rates which are correct to order B^2 the cross sections *used to compute these reaction rates* cannot be buckling independent. We see no way to circumvent this difficulty. Further the quantities $D_x^{(\lambda)} B_x^2 \phi$ and $D_y^{(\lambda)} B_y^2 \phi$ are not simply leakage rates since $D^{(\lambda)}$ contains, implicitly, contributions due to the buckling dependence of $\nu \Sigma_f$ and Σ_a. It is possible that the use of such a diffusion coefficient is not appropriate near interfaces. On the other hand, there seems to be no good

theoretical foundation for any homogenization prescription near inter-
faces. Clearly, then, we cannot claim to have solved all the problems
involved in the computation of homogenized group constants. Yet, despite
all the remaining difficulties, it still seems important to require that
a homogenization procedure should preserve the heterogeneous eigenvalue,
in an infinite lattice, to order B^2.

In closing we note that much of what has been said here is obviously
relevant in other geometries, as well as in slab geometry. Clearly our
arguments about eigenvalues and reaction rates are equally valid in any
periodic lattice. Perhaps it is not quite so obvious that the Benoist
and Bonalumi diffusion coefficients are generally double-valued in square
and hexagonal cells, just as they are in slab cells. Yet this is true.
Consider, for example, an array of rods in a square or hexagonal lattice.
It is customary (and convenient) to define a unit cell with the rod at
its center: but it is also possible to define a cell with a rod at each
corner of its boundary. Corresponding to each of these two possible
definitions of the unit cell we would get two values of the exact Benoist
diffusion coefficient, and two values of the Bonalumi coefficients.

REFERENCES AND FOOTNOTES

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[4]R. A. BOUNALUMI, *Energ. Nucl. (Milan)*, **18**, 395 (1971).

[5]D. MENEGHETTI, "Recent Advances and Problems in Theoretical Analyses of ZPR-III Fast Critical Assemblies," in *Physics of Fast and Intermediate Reactors*, International Atomic Energy Agency, Vienna, p. 457.

[6]The substitutions made in Eqs. (2), (3), and (4) are of a form attributed to Brissenden by M. M. R. Williams, *Atomkernenergie*, **18**, 31 (1971) Lfg. 1.

[7]The reader may observe that $\int d\hat{\Omega} \; I^{(0.1)}$ vanishes and we make use of this fact later.

[8]The definition of x_L and x_R will be discussed further in Section III.

[9]See, for example, Ref. 3, Eq. (A-15).

[10]Since $j_{1,11}$ and ϕ are periodic we may take, as the value of x_B, either x_L or x_R.

[11]D. A. SELENGUT, "Diffusion Coefficients for Heterogeneous Systems," Nuclear Physics Research Quarterly, HW-60220 (1959), p. 65.

[12]W. W. ENGLE, JR., "A User's Manual for ANISN, A One-Dimensional Discrete Ordinates Transport Code with Anisotropic Scattering," K-1693, Union Carbide Corporation, Nuclear Division (1967), contained in CCC-92, Radiation Shielding Information Center.

[13]Note that this is not the "anisotropic effect" defined, for example, in Ref. 4. The anisotropy effect as usually defined contains, in fact, only part of the true effects due to anisotropy in the flux.

[14]M. M. R. WILLIAMS, *Atomkernenergie*, **18**, 31 (1971) Lfg. 1.

TABLE I

Test Problem Parameters

(Left- and right-hand boundaries are symmetry planes.
Source density has been set equal to $\nu\Sigma_f$ in each region.)

	Region I (Uranium Oxide)	Region II (Sodium)	Region III (Uranium-Plutonium)
Thickness (cm)	1.0	1.25	0.25
Source Density	0.00998	0.	0.185
Σ_t	0.181551	0.0452915	0.252648
Σ_{s0}	0.117890	0.0267661	0.0860426

TABLE II

Parallel Diffusion Coefficients
in a Typical ZPPR Lattice

	DP_3-P_7	DP_4-P_9	DP_5-P_{11}
D_2 (cm)	2.8705	2.8740	2.8768
	DP_3-P_0	DP_4-P_0	DP_5-P_0
$\hat{D}_2$ (cm)	2.8613	2.8707	2.8798

D_2 is computed from Eqs. (12), (36), and (39).

$\hat{D}_2$ is the Benoist approximate D_2, computed from Eqs. (12), (13'), and (36').

TABLE III

Diffusion Coefficients Normal to Plates

	$DP_3 - P_7$	$DP_4 - P_9$	$DP_5 - P_{11}$
$\bar{\bar{D}}_1$	2.759	2.765	2.769
	$DP_3 - P_0$	$DP_4 - P_0$	$DP_5 - P_0$
$\bar{D}_1$	2.772	2.771	2.771

$\bar{\bar{D}}_1$ is computed from Eqs. (14) and (35"'):
anisotropic source term $\mu R^{(0,0)}$.

$\bar{D}_1$ is computed from Eqs. (14") and (35"):
isotropic source term $\mu\phi$.

TABLE IV

Coefficients for Diffusion Normal
to Plates, According to Benoist's
and Bonalumi's Prescriptions

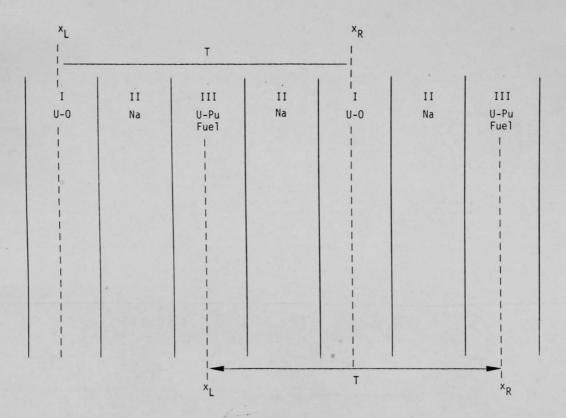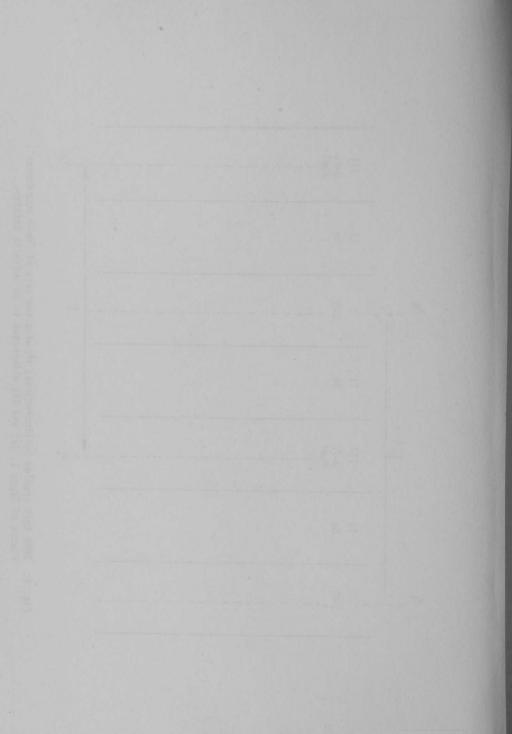| D_1 from Benoist's Definitions		
$D_1^A\left(x_B\right)$	$D_1^B\left(x_B\right)$	$\hat{D}_1$
DP_5	DP_5	DP_5
2.7775	2.7211	2.7677
$D_1^A\left(x_B\right)$	$D_1^B\left(x_B\right)$	
DP_5	DP_5	
source = $\mu\phi$	source = $\mu\phi$	
2.7754	2.7460	
D_1 from Bonalumi's Definition		
$D_1^A\left(x_B\right)$	$D_1^B\left(x_B\right)$	
DP_5	DP_5	
2.9182	2.4378	

Fig. 1. ZPPR test problem configurations, showing two sets of "cell boundaries". Plates of Types I, II, and III alternates in an infinite lattice.